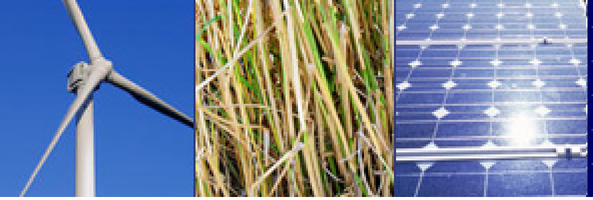

Renewable Electricity – Solar Energy Conversion

September 20, 2007

Second Plenary

Panel Members

- Sam Baldwin
- Victor Batista
- Miroslav Begovic
- Jerry Bernholc
- Rana Biswas
- Gang Chen
- Lori Diachin
- Phillip Duxbury
- James Evans
- George Fann
- Al Geist
- Peter Graf
- Kai-Ming Ho
- Roy Hogan
- Mark Hybertsen
- Gary Johnson
- Yosuke Kanai
- Efthimios Kaxiras
- Shawn Lin
- Dmitry Matyushov
- Jeffrey Mazer
- James Misewich
- Jayathi Murthy
- Jeffrey Neaton
- Ruth Pachter
- Roger Pawlowski
- Mark Pederson
- Joerg Petrasch
- Angus Rockett
- Andy Salinger
- Andrew Shabaev
- G. Malcolm Stocks
- Dallas Trinkle
- Lin-Wang Wang
- Shengbai Zhang
- Yong Zhang

Priority Research Directions

- Defects, grain boundaries & alloys of inorganic semiconductors.
- Polymeric & small molecule organics; nanostructured composites (nano-organics mixes)
- Complex, hybrid materials systems (thermoelectrics, interfaces, biomimetic systems)
- Component simulation methods: Integration of physics based models to simulate & optimize light management, carrier generation & carrier transport to predict performance of multi-component photovoltaic systems
- Process simulation methods: Efficient, robust computational techniques for atomistic to continuum, multi-time scale, multi-physics simulation of materials processing and assembly for solar energy applications.

Materials Optimization in Inorganic PV

Challenges

* Current inorganic PV are either cheap or efficient, but not both

* Defects are often the limiting factor (recombination at defect sites or grain boundaries, decreased mobility, material instabilities)

Summary of Research Direction

* Computational predictions of defect thermodynamics, stability, diffusion, energy levels, generation mechanisms
* Doping efficiency vs recombination
• Band gap engineering – alloying
• Transport, interfaces & grain boundaries

Needs from Computational Science

• Methods for accurate determination of gap and defect levels, many-body effects

• Structure determination of large systems – reduced scaling methods

• Better local (electronic structure) and global (atomic structure) minimization methods

• Petascale parallelization & load optimization

Potential Impact on Solar Energy

• High efficiency (close to thermodynamic limit), cheap (defect-tolerant) solar cells

• Feed forward to device simulation and pilot projects: comparison to experiment

Research impact – 5 years

Production impact – 8 years

Organic Polymerics & Small Molecules and Inorganic Nanostructure PVs

Challenges

While cheap, the current PV cells made of these materials suffer low efficiency and degradation:

- Exciton transport and dissociation
- Carrier transport and collection
- Electronic structure, optical property and carrier dynamics in nanosystems
- Mechanism of radiation induced degradation.

Summary of Research Direction

•Charge separation and recombination process in organic/nano systems
•Excited state and exciton binding energies
•Electronic structure of nanoparticles, the PV effects of traps and surface states, and multiple exciton generation

Needs from Computational Science

•Aperiodic methods scalable for large number procedures.
•More accurate methods for excited states
•Order-N large-scale electronic structure methods for nanosystems
•Computational methods for charge transport in complex/disordered systems
•Better model for reactivities of photoexcited systems

Potential Impact on Renewable Energy

•Realistic model and quantitative understanding of the carrier generation and dynamics processes.
•Rational design for more efficient and stable 3rd-generation PV
•Research Impact 7 years
•Production Impact 10 years

Design And Optimization of Complex, Biomimetic and Hybrid Materials for Solar-Electric Energy Conversion

Challenges

- Lack of reliable, effective computational tools for predicting structure, excited states, and thermal/electrical transport properties of complex, biomimetic and hybrid photovoltaic and thermoelectric materials.

Needs from Computational Science

- Efficient, long time *ab initio* based molecular methods.
- Reliable calculations of thermal conductivity.
- Techniques for electronic transport in complex materials – defect scattering and electron phonon calculations.
- Modeling stability and formation of nanostructures and their effect on energy conversion efficiency.
- Calculating open circuit voltage, e^--h^+ separation rates, carrier trapping dynamics and exciton kinetics, photo-absorption properties, interfacial injection and electronic and thermal relaxation.

Summary of Research Direction

- Computational predictions of photon conversion, charge and thermal transport in complex and nanostructured bulk materials and interfaces of biomimetic and hybrid systems.
- Structural prediction and stability assessment.
- Impact of structural defects, disorder and surface passivation in nanoscale heterogeneity.
- Development of new methodologies for electrical and thermal conductivity.

Potential Impact on Renewable Energy

- Provide fundamental insight for the development of a new generation of photovoltaic materials.
- Development of a direct solar thermal to electricity approach.
- Advancing our understanding on the effect of structure and chemistry on thermal and electrical transport leading efficiency breakthroughs (tools for research use 2-3 years, materials discovery 3-5 years).

Integrated Physics-Based Simulation and Optimization of Multi-Component Photovoltaic Systems

Challenges

- Validated prediction, design, & optimization of photovoltaic system performance.
- Integrated treatment of light harvesting, charge separation & carrier collection.
- Assessment of PV device performance with breakthrough materials & architectures.

Summary of Research Direction

- Pilot device concepts: e.g. intermediate band solar cells, high internal surface area organic PV devices, light harvesting systems, multiple-exciton generation materials.
- Developing integration approaches for physical models: Maxwell, transport, kinetics

Needs from Computational Science

- New multi-scale Maxwell solvers to handle near-field plasmonic effects out to the far-field for photon harvesting.
- Stable algorithms for solution of the non-linear coupled equations from physical models.
- Algorithms for hierarchical optimization over complex and large design spaces.

Potential Impact on Solar Energy

- Optimizing performance of targeted current PV designs through collaboration (4 years).
- Extensible software for use by PV device designer engineers (6 years).
- Realizing promise of third generation PV materials in device architectures (8 years).

Processing Simulations for PV Materials Manufacturing

Challenges

•Linking manufacturing process to material characteristics and performance for efficient solar energy conversion.

•Simulation of novel heterogeneous manufacturing techniques and heterogeneous flowchart modeling. i.e. nanostructure deposition, large-scale self assembly, sol-gel etc...

Summary of Research Direction

•Develop robust and scalable algorithms to enable atomistic to continuum, multi-timescale, multi-physics, modeling of materials processing.

- –Reactor scale CVD, PVD and crystal melt growth of poly/amorphous Si linked to electronic structure, MD and statistical mechanics.
- –Nucleation/growth of grains in poly-crystalline thin films.

•Validation of models with experimental data.

Needs from Computational Science

•Scalable tools for large scale Eigen-system analysis, fast order-n methods, and high-dimensional phase-space analysis

•Multi-objective optimization and inverse parameter estimation for hetergeneous processing

•Mathematically rigorous multi-physics coupling

•Multi-scale stochastic quantum dots for thermodynamics for large area self assembly

Potential Impact on Solar Energy

•Accelerate the product development cycles

•Facilitate the transition of development processes centered on the costly “cook and look” approach to an efficient science based “know and grow” approach.

•Facilitate laboratory-scale to fabrication-scale transition of emerging solar technology.

•Impact will be felt in 5 – 10 years